

Sampler algorithm for non-convex inverse problem

Pierre Palud

PhD directed by
Pierre Chainais, Franck Le Petit

with the collaboration of
Emeric Bron, Pierre-Antoine Thouvenin

Ecole Centrale de Lille, CRIStAL, LERMA

financed by CNRS via 80|Prime



Solar systems fill $\sim 3 \cdot 10^{-10}$ of the volume of the galaxy

~~Most of the galaxy: empty!~~

Most of the galaxy: **Interstellar Medium!**

Observations of GMC: Orion B in visible frequencies



Figure: Image from Pety et al. [2016]

Observations of GMC: Orion B in visible frequencies

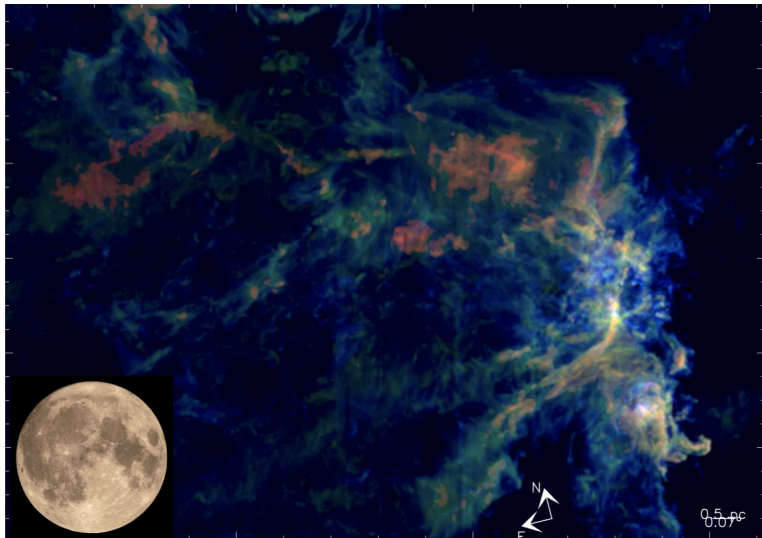


Figure: Image from Pety et al. [2016]
blue: ^{12}CO , green: ^{13}CO , red: C^{18}O

Photo-Dissociation Region (PDR)

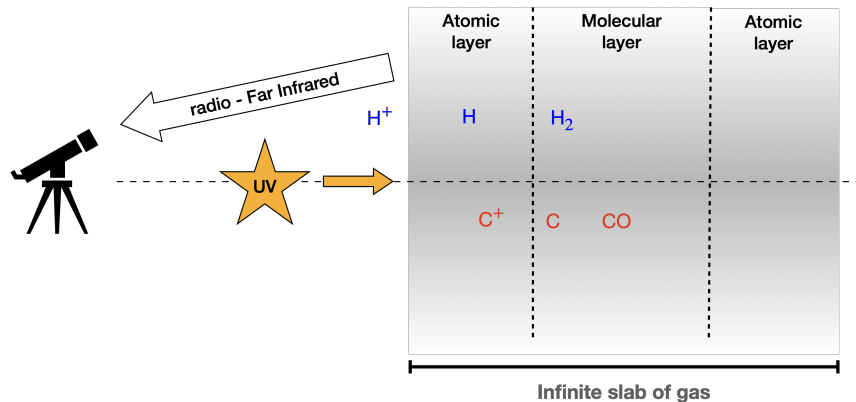


Figure: Structure of a PDR

Photo-Dissociation Region (PDR)

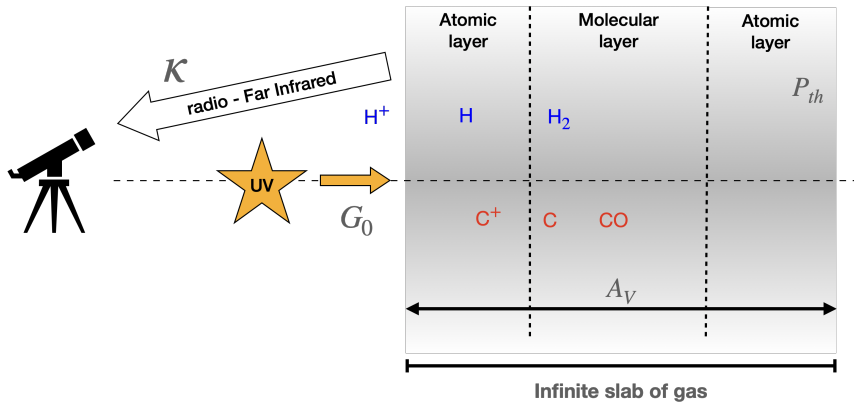
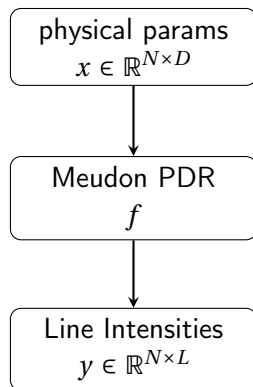


Figure: Structure of a PDR

Meudon PDR code: numerical simulation of a PDR

- Introduced in Le Petit et al. [2006].
- for stationary 1D slab of gas, solves:
 - 1 radiative transfer
 - 2 chemistry
 - 3 thermal balancethat are all **coupled!**



Can we infer x from y and f ?
no ground truth → with credibility intervals

Current state of the art in astrophysics

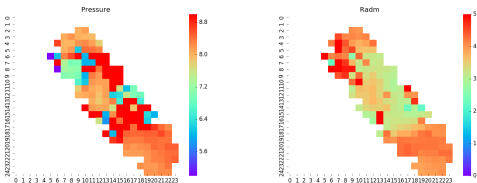
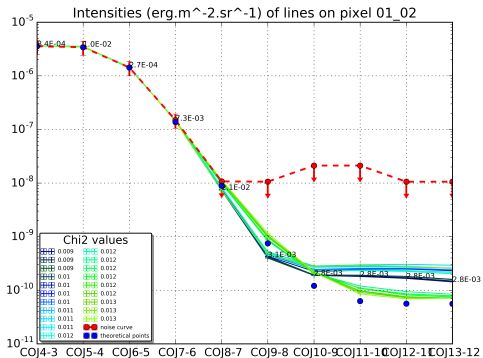


Figure: MLE maps inference

inference with credibility interval



a posteriori probability distribution $\mathbb{P}[x | y]$

$$\underbrace{\mathbb{P}[x | y]}_{\text{a posteriori}} \propto \underbrace{\mathbb{P}[y | x]}_{\text{likelihood}} \times \underbrace{\mathbb{P}[x]}_{\text{a priori}}$$

Complex distribution

⇒ impossible to manipulate as is

⇒ sampling with **MCMC**

Observation model

$$\forall n, \ell, y_{n,\ell} = \max \left\{ \omega, \epsilon_{n,\ell}^{(m)} f_{\ell}(x_n) + \epsilon_{n,\ell}^{(a)} \right\}$$

with

- $\epsilon_{n,\ell}^{(a)}$: additive noise (thermal, instruments)
- $\epsilon_{n,\ell}^{(m)}$: multiplicative noise (calibration error)
- ω : minimum detectable value by telescope

Observation model

$$\forall n, \ell, y_{n,\ell} = \max \left\{ \omega, \epsilon_{n,\ell}^{(m)} f_{\ell}(x_n) + \epsilon_{n,\ell}^{(a)} \right\}$$

with

- $\epsilon_{n,\ell}^{(a)}$: additive noise (thermal, instruments)
- $\epsilon_{n,\ell}^{(m)}$: multiplicative noise (calibration error)
- ω : minimum detectable value by telescope

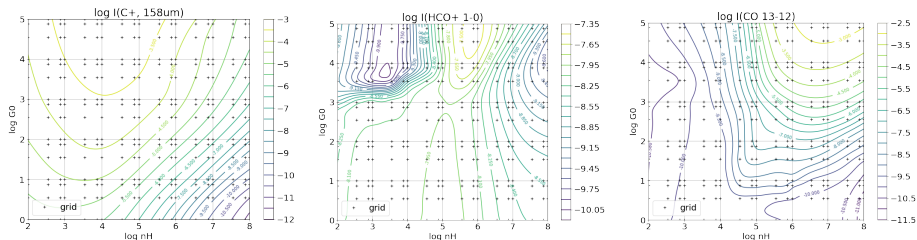


Figure: f_{ℓ} for some lines ℓ , for 1 pixel

a priori information on x :

- spatial regularization: L2 penalty on image Laplacian
- f_ℓ : estimated from a grid
 - **constraint of belonging to a cube** (convex envelope of grid)
 - ⚠ non smooth prior ⚠ but can be tempered with a smooth penalty

smooth prior + **smooth** likelihood \implies **smooth** posterior
classic **MCMC algorithm** (e.g., MALA) OK

smooth prior + **smooth** likelihood \Rightarrow **smooth** posterior
classic ~~MCMC algorithm~~ (e.g., MALA) OK because of two difficulties

smooth prior + **smooth** likelihood \Rightarrow **smooth** posterior
classic ~~MCMC algorithm~~ (e.g., MALA) OK because of two difficulties

- f and ∇f cover **various decades**
 \Rightarrow classic methods **inefficient**

smooth prior + **smooth** likelihood \Rightarrow **smooth** posterior
classic ~~MCMC algorithm~~ (e.g., MALA) OK because of two difficulties

- f and ∇f cover **various decades**
 \Rightarrow classic methods **inefficient**
- **non-convex** negative log-posterior (because of Meudon PDR code)
 \Rightarrow need to avoid being **trapped in local minima**

smooth prior + **smooth** likelihood \Rightarrow **smooth** posterior
classic ~~MCMC algorithm~~ (e.g., MALA) OK because of two difficulties

- f and ∇f cover **various decades**
 - \Rightarrow classic methods **inefficient**
 - ✓ **Preconditioned MALA kernel with RMSProp**
- **non-convex** negative log-posterior (because of Meudon PDR code)
 - \Rightarrow need to avoid being **trapped in local minima**
 - ✓ **Multiple-Try Metropolis (MTM) kernel**

smooth prior + **smooth** likelihood \Rightarrow **smooth** posterior
classic ~~MCMC algorithm~~ (e.g., MALA) OK because of two difficulties

- f and ∇f cover **various decades**
 \Rightarrow classic methods **inefficient**
✓ **Preconditioned MALA kernel with RMSProp**
- **non-convex** negative log-posterior (because of Meudon PDR code)
 \Rightarrow need to avoid being **trapped in local minima**
✓ **Multiple-Try Metropolis (MTM) kernel**

Final sampler : random combination of these two kernels

Illustration: Gaussian Mixture in a square

Illustration that our algorithm explores interesting **local minima** :

- mixture of 20 gaussians
- with constraint $x \in [-10, 10] \times [-10, 10]$

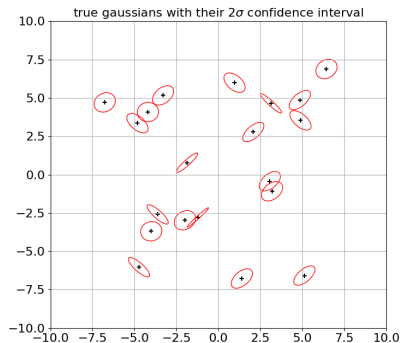
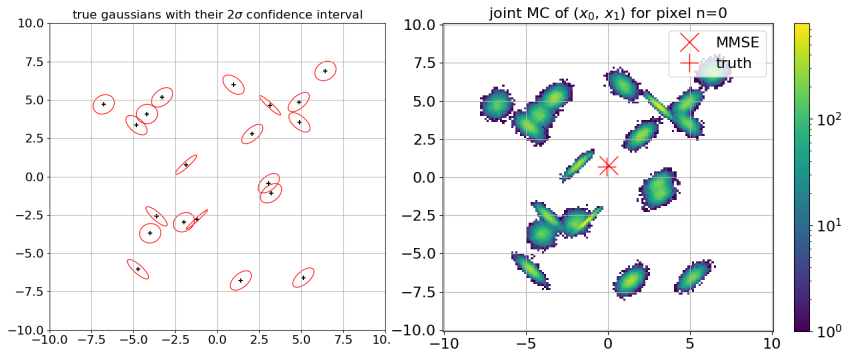


Illustration: Gaussian Mixture in a square

Illustration that our algorithm explores interesting **local minima** :

- mixture of 20 gaussians
- with constraint $x \in [-10, 10] \times [-10, 10]$



Toy case 1: Time Series Inversion

$$y_{n,\ell} = \epsilon_{n,\ell}^{(m)} f(x_n) + \epsilon_{n,\ell}^{(a)} \text{ with } f: x \in \mathbb{R} \mapsto e^x, \sigma_a = 1, \sigma_m \sim 10\%$$

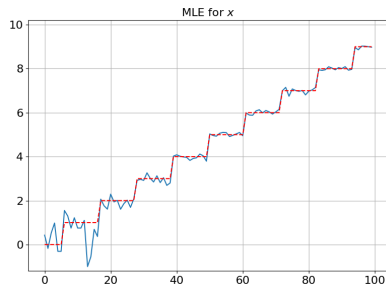
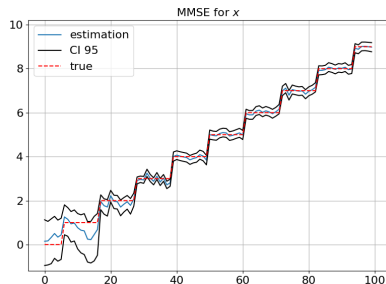
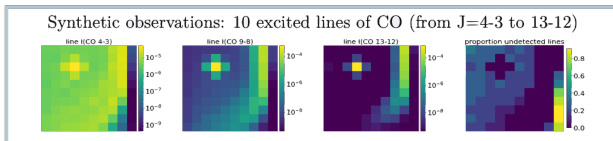
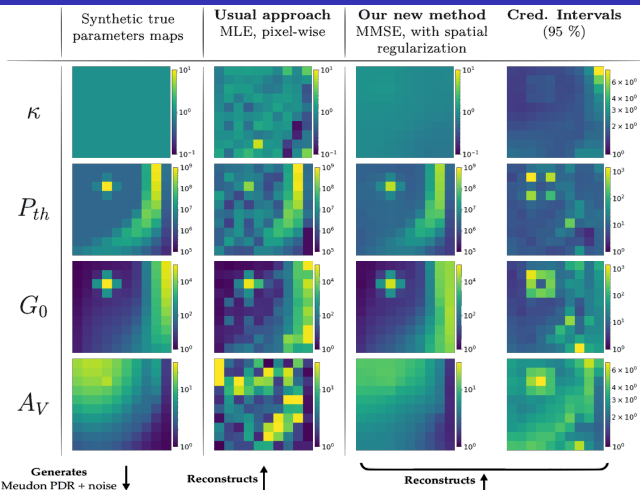


Table: Estimation Summary

estimator	MSE	SNR
MMSE	3.6	28.8
MLE	10.5	24.1

Astrophysical Toy case: Map Inversion



Application to NGC 7023 (1 pixel)

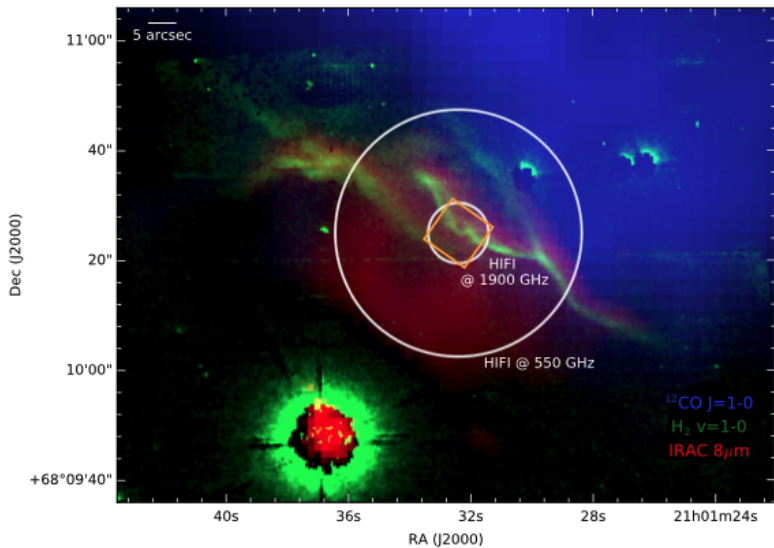
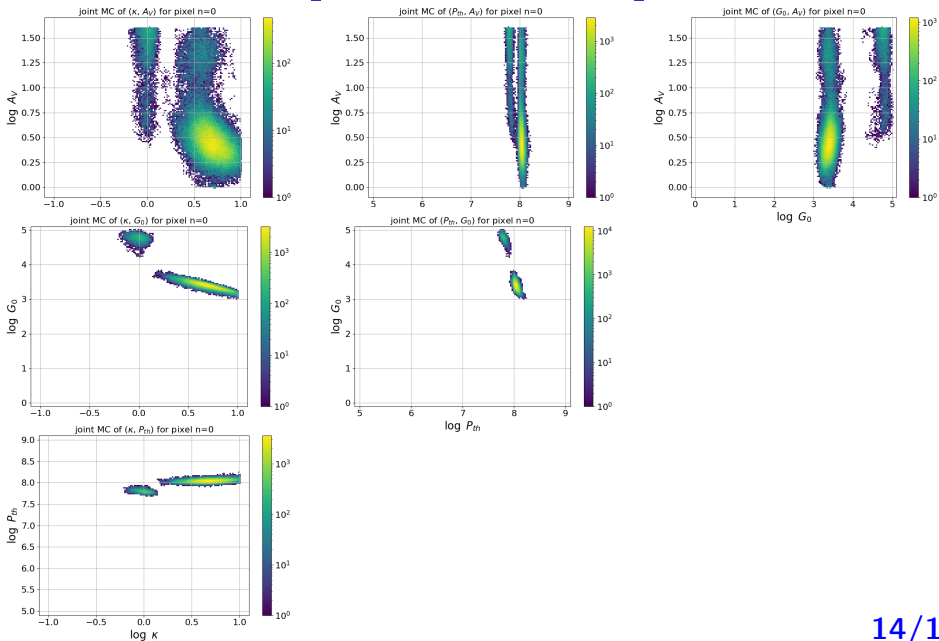


Figure: from Joblin et al. [2018]

Application to NGC 7023 (1 pixel)



- Definition of a MCMC sampler with
 - 1 P-MALA kernel to tackle regularity issues
 - 2 MTM kernel to tackle the non-log-concavity of the posterior
- Evaluation of the method on toy data
- Application to real world data

Thank you for your attention!



- C. Joblin, E. Bron, C. Pinto, P. Pilleri, F. Le Petit, M. Gerin, J. Le Bourlot, A. Fuente, O. Berne, J. R. Goicoechea, E. Habart, M. Köhler, D. Teyssier, Z. Nagy, J. Montillaud, C. Vastel, J. Cernicharo, M. Röllig, V. Ossenkopf-Okada, and E. A. Bergin. Structure of photodissociation fronts in star-forming regions revealed by *Herschel* observations of high-J CO emission lines. *Astronomy & Astrophysics*, 615:A129, July 2018. ISSN 0004-6361, 1432-0746. doi: 10.1051/0004-6361/201832611. URL <https://www.aanda.org/10.1051/0004-6361/201832611>.
- F. Le Petit, C. Nehme, J. Le Bourlot, and E. Roueff. A Model for Atomic and Molecular Interstellar Gas: The Meudon PDR Code. *The Astrophysical Journal Supplement Series*, 164(2):506–529, June 2006. ISSN 0067-0049, 1538-4365. doi: 10.1086/503252. URL <https://iopscience.iop.org/article/10.1086/503252>.

- J. Pety, V. Guzman, J. Orkisz, H. Liszt, M. Gerin, E. Bron, S. Bardeau, J. Goicoechea, P. Gratier, F. Petit, F. Levrier, K. Oberg, E. Roueff, and A. Sievers. The anatomy of the Orion B Giant Molecular Cloud: A local template for studies of nearby galaxies. *Astronomy & Astrophysics*, 599, Nov. 2016. doi: 10.1051/0004-6361/201629862.